

James R. Faeder, Ph.D.

Technical Staff Member

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Education

- Ph.D. in Chemical Physics, University of Colorado, 1998.
- A.B., summa cum laude, in Chemistry, Harvard College, 1991.
- High school, Norfolk Academy, 1987.

Awards and Honors

- Director-funded Postdoctoral Fellow at Los Alamos National Laboratory, 2001-2003.
- Feinberg Postdoctoral Fellowship at the Weizmann Institute of Science, 1999-2001.
- NSF travel award to attend CECAM conference on Instantaneous Normal Modes in Lyon, France, July, 1999.
- Teresa Fonseca Prize for outstanding research in theoretical chemistry at the University of Colorado, 1997.
- National Science Foundation Graduate Research Fellowship, 1992-1995.
- University of Colorado Graduate Fellowship, 1991-1992.
- Phi Beta Kappa, Harvard College, 1991.
- ICI Summer Research Fellowship, 1991.
- National Merit Scholar, 1987-88.
- Bethel Science Scholarship from the Virginia Junior Academy of Science, 1987.

Research Experience

- July, 2003- Technical Staff Member in the Theoretical Biology and Biophysics Group, Los Alamos National Laboratory.
Projects include developing models of receptor-mediated signaling in the immune system.
- 2001-2003 Postdoctoral Fellow in the Theoretical Biology and Biophysics Group, Los Alamos National Laboratory.
A member of the Cell Signaling Team, developing detailed, molecular level models of cell signaling cascades in the immune system.
- 1999-2001 Postdoctoral Fellow with Prof. D. Tannor, Department of Chemical Physics, Weizmann Institute of Science.
Theory and simulation of nonlinear optical spectroscopy and coherent control from the gas phase to the condensed phase (in collaboration with Prof. Y. Prior).
- 1998-1999 Postdoctoral Associate with Prof. B. Ladanyi, Department of Chemistry, Colorado State University.
Molecular dynamics simulations of the interior of aqueous reverse micelles (in collaboration with Prof. N. Levinger).
- 1992-1998 Research Assistant, with Prof. R. Parson, JILA and Department of Chemistry and Biochemistry, University of Colorado.
Modeling structure and photodissociation dynamics of molecular ions in clusters (in collaboration with Prof. W.C. Lineberger).

- Summer, 1991 Summer Research Assistant with Dr. A. Burgess, Research Division, ICI, Runcorn Heath, UK.
Molecular dynamics simulations of small fluorocarbons for comparison with neutron diffraction experiments.
- 1990-1991 Undergraduate Research Assistant with Prof. W. Klemperer, Department of Chemistry, Harvard University.
Microwave spectroscopy of weakly bound molecular clusters.

Teaching Experience

- Summer, 2002 Research Advisor for Los Alamos Summer School, Los Alamos National Laboratory.
Directed research project on developing new representations of cell signaling cascades by undergraduate student Jeremy Kozdon.
- Summer, 1999 Research Advisor for Summer Undergraduate Theory Program, Department of Chemistry, Colorado State University.
Directed research project on reverse micelle simulations by student M. Albert.
- 1991-1992 Teaching Assistant for General Chemistry, University of Colorado.
Duties involved recitations, directing labs, grading homework, and conducting review sessions.

Professional Affiliations

Member of the American Chemical Society since 1996.

Member of the American Physical Society since 1998.

Member of the American Association of Immunologists since 2003.

Professional Service

Reviewer for journals *J. Chem. Phys.*, *Bioessays*, *J. Theor. Biol.*, and *Complexity*.

Peer-Reviewed Publications

1. A. L. Cooksy, S. Drucker, J. Faeder, and W. Klemperer. "High resolution spectrum of the $v=1$ Π state of ArHCN." *J. Chem. Phys.*, **95**, 3017, 1991. ([pdf](#))
2. J. Faeder. "A distributed Gaussian approach to the vibrational dynamics of Ar-benzene." *J. Chem. Phys.*, **99**, 7664, 1993.
3. P. E. Maslen, J. M. Papanikolas, J. Faeder, R. Parson, and S. V. O'Neil. "Solvation of electronically excited I_2^- ." *J. Chem. Phys.*, **101**, 5731, 1994.
4. P. E. Maslen, J. Faeder, and R. Parson. "Ab initio calculations of the ground and excited states of I_2^- and ICl^- ." *Chem. Phys. Lett.*, **263**, 63-72, 1996. ([pdf](#))
5. J. Faeder, N. Delaney, P. Maslen, and R. Parson. "Charge flow and solvent dynamics in the photodissociation of cluster ions: A nonadiabatic molecular dynamics study of $I_2^- \cdot Ar_n$." *Chem. Phys. Lett.*, **270**, 196-205, 1997. ([pdf](#))
6. N. Delaney, J. Faeder, P. E. Maslen, and R. Parson. "Photodissociation, recombination and electron transfer in cluster ions: A nonadiabatic molecular dynamics study of $I_2^-(CO_2)_n$." *J. Phys. Chem. A*, **101**, 8147-8151, 1997. ([pdf](#))
7. J. Faeder and R. Parson. "Ultrafast reaction dynamics in cluster ions: Simulation of the transient photoelectron spectrum of $I_2^- Ar_n$ photodissociation." *J. Chem. Phys.*, **108**, 3909-3914, 1998. ([pdf](#))

8. S. Nandi, A. Sanov, N. Delaney, J. Faeder, R. Parson, and W. C. Lineberger. "Photodissociation of $I_2^-(OCS)_n$ cluster ions: Structural implications." *J. Phys. Chem. A*, **102**, 8827-8835, 1998. ([pdf](#))
9. P. E. Maslen, J. Faeder, and R. Parson. "An effective Hamiltonian for an electronically excited solute in a polarizable molecular solvent." *Mol. Phys.*, **94**, 693-706, 1998. ([pdf](#))
10. J. Faeder, N. Delaney, P. E. Maslen, and R. Parson. "Modeling structure and dynamics of solvated molecular ions: Photodissociation and recombination in $I_2^-(CO_2)_n$." *Chem. Phys.*, **239**, 525-547, 1998. ([pdf](#))
11. N. Delaney, J. Faeder, and R. Parson. "Photodissociation and recombination of solvated I_2^- : What causes the transient absorption peak?" *J. Chem. Phys.*, **111**, 452-455, 1999. ([pdf](#))
12. N. Delaney, J. Faeder, and R. Parson. "Simulation of UV photodissociation of $I_2^-(CO_2)_n$: Spin-orbit quenching via solvent mediated electron transfer." *J. Chem. Phys.*, **111**, 651-663, 1999. ([pdf](#))
13. A. Sanov, J. Faeder, R. Parson, and W. C. Lineberger. "Spin-orbit coupling in $I\cdot CO_2$ and $I\cdot OCS$ van der Waals complexes: beyond the pseudo-diatomic approximation." *Chem. Phys. Lett.*, **313**, 812-819, 1999. ([pdf](#))
14. J. Faeder and B. M. Ladanyi. "Molecular dynamics simulations of the interior of aqueous reverse micelles." *J. Phys. Chem. B*, **104**, 1033-1046, 2000. ([pdf](#))
15. R. Parson, J. Faeder, and N. Delaney. "Charge flow and solvent dynamics in the photodissociation of solvated molecular ions" (Feature Article). *J. Phys. Chem. A*, **104**, 9653-9665, 2000. ([pdf](#))
16. J. Faeder and B. M. Ladanyi. "Solvation dynamics in aqueous reverse micelles: A computer simulation study." *J. Phys. Chem. B*, **105**, 11148-11158, 2001. ([pdf](#))
17. J. Faeder, I. Pinkas, G. Knopp, Y. Prior, and D. J. Tannor. "Vibrational Polarization Beats in Femtosecond CARS: A Signature of Dissociative Pump-Dump-Pump Wavepacket Dynamics." *J. Chem. Phys.*, **115**, 8440-8454, 2001. ([pdf](#))
18. B. Goldstein, J. R. Faeder, W. S. Hlavacek, M. L. Blinov, A. Redondo, and C. Wofsy. "Modeling the early signaling events mediated by aggregation of FcεRI." *Mol. Immunol.*, **38**, 1213-1219, 2002. ([pdf](#))
19. J. Faeder, M. V. Albert, and B. M. Ladanyi. "Molecular dynamics simulations of the interior of aqueous reverse micelles: A comparison between sodium and potassium counterions." *Langmuir*, **19**, 2514-2520, 2003. ([pdf](#))
20. J. R. Faeder, W. S. Hlavacek, I. Reischl, M. L. Blinov, H. Metzger, A. Redondo, C. Wofsy, and B. Goldstein. "Investigation of early events in FcεRI-mediated signaling using a detailed mathematical model." *J. Immunol.*, **170**, 3769-3781, 2003. ([pdf](#))
21. W. S. Hlavacek, J. R. Faeder, M. L. Blinov, A. S. Perelson, B. Goldstein. "The complexity of complexes in signal transduction." *Biotechnol. Bioeng.*, **84**, 783-794, 2003. ([pdf](#))
22. B. Goldstein, J. R. Faeder, and W. S. Hlavacek. "Mathematical and computational models of immune-receptor signalling." *Nat. Rev. Immunol.*, **4**, 445-456, 2004 ([pdf](#)).
23. M. L. Blinov, J. R. Faeder, B. Goldstein, and W. S. Hlavacek, "BioNetGen: software for rule-based modeling of signal transduction based on the interactions of molecular domains." *Bioinformatics*, in press, 2004 ([pdf](#)).
24. J. R. Faeder, M. L. Blinov, B. Goldstein, and W. S. Hlavacek. "Combinatorial complexity and dynamical restriction of network flows in signal transduction." Submitted.

Other Publications

1. W. C. Lineberger, M. Nadal, P. Campagnola, V. Vorsa, P. D. Kleiber, J. M. Papanikolas, P. E. Maslen, J. Faeder, R. Parson, and O. E. Poplawski. "Time-resolved dynamics in large cluster ions." In *Proceedings of the Robert A. Welch Foundation 38th Conference on Chemical*

Research: Chemical Dynamics of Transient Species, Houston, Texas, 1994. R. A. Welch Foundation.

2. R. Parson and J. Faeder. "Ultrafast reaction dynamics in molecular cluster ions." *Science*, **276**, 1660, 1997. ([link](#))
3. J. Faeder. *The X_2^- files: Modeling photodissociation of molecular ions in clusters*. PhD thesis, University of Colorado at Boulder, 1998. ([pdf](#) | [GZipped PS](#))
4. M. L. Blinov, J. R. Faeder, and W. S. Hlavacek (2003). *Software and procedures for creating mathematical/computational models of cellular signaling*. US Patent Application S-100,635.

Conference Participation and Invited Talks

1. Poster presentation, "A model for the structure and dynamics of solvated molecular ions," *Conference on the Dynamics of Molecular Collisions*, Asilomar, California, July, 1995.
2. Poster presentation, "Structure and dynamics of solvated molecular ions," *American Conference on Theoretical Chemistry*, Park City, Utah, July, 1996.
3. Contributed talk, "Charge flow and solvent dynamics in the photodissociation of cluster ions," *Annual Meeting of the American Chemical Society*, Las Vegas, Nevada, August, 1997.
4. Invited talk, "Modeling water structure and dynamics inside a reverse micelle," and contributed talk, "Simulations of $\text{ICl}(\text{CO}_2)_n$ photodissociation: Role of structure and excited state charge flow," *Centennial Meeting of the American Physical Society*, Atlanta, Georgia, March, 1999.
5. Participant, *CECAM Workshop on Instantaneous Normal Modes*, Lyon, France, July, 1999.
6. Poster presentations, "Simulations of $\text{ICl}(\text{CO}_2)_n$ photodissociation" and "Modeling water structure and dynamics inside a reverse micelle," *American Conference on Theoretical Chemistry*, Boulder, Colorado, July, 1999.
7. Invited lecture, "Structure and dynamics of water in reverse micelles", *Physical Chemistry Seminar*, Hebrew University, Jerusalem, Israel, May, 2000.
8. Contributed talk, "Photodissociation dynamics of molecular cluster ions," *Gordon Graduate Summer School on Analytical Theory*, Bristol, Rhode Island, June, 2000.
9. Poster presentation, " $\text{ICl}(\text{CO}_2)_n$ photodissociation: Effects of structure, excited state charge flow, and solvent dynamics," *Faraday Discussion on Cluster Dynamics*, Durham, England, April, 2001.
10. Poster presentation, "A detailed kinetic model of immunoreceptor signaling", *The Second International Conference on Systems Biology*, Pasadena, California, November, 2001.
11. Poster selected for oral presentation, "A mathematical model for the activation of Syk through the Fc ϵ RI signaling complex", *FASEB Summer Research Conference on Immunoreceptors*, Tucson, Arizona, August, 2002.
12. Invited talk, "Modeling immunoreceptor signaling: A detailed study of Fc ϵ RI," *Workshop on Enabling Concepts in Biosystems Analysis*, Santa Fe, New Mexico, September, 2002.
13. Poster selected for oral presentation, "Mathematical modeling of early events in Fc ϵ RI-mediated signaling", *The American Association of Immunologists 90th Anniversary Meeting*, Denver, Colorado, May, 2003.
14. Poster presentation, "Combinatorial complexity in receptor signaling," The 23rd Annual Conference of the Center for Nonlinear Studies at Los Alamos National Laboratory, Santa Fe, New Mexico, May, 2003.
15. Poster selected for oral presentation, "Combinatorial complexity in immunoreceptor signaling", *FASEB Summer Research Conference on Signal Transduction in the Immune System*, Snowmass, CO, June, 2003.
16. Poster presentation, "Networks That Govern Complex Formation during Signal Transduction Exhibit Narrow Flows", *The Fourth International Conference on Systems Biology*, St. Louis, Missouri, November, 2003. ([abstract-pdf](#))

17. Invited talk, "Modeling Complex Formation in Signal Transduction What we've learned so far," *Second New Mexico Workshop on Computational Cell Biology*, Santa Fe, New Mexico, January, 2004.
18. Invited lecture, "Mathematical Models of Cell Signaling: Complex Complexes", University of New Mexico Biocomplexity Seminar Series, Albuquerque, New Mexico, February, 2004.
19. Poster presentation, "Modeling combinatorial complexity in cell signaling", *Mathematical Models in Signaling Systems*, Vanderbilt University, Nashville, Tennessee, June, 2004.
20. Abstract selected for oral presentation, "Investigating the Role of Complex Formation in Immunoreceptor Signaling Using Mathematical Modeling," *12th International Congress of Immunology and the 4th Annual Meeting of FOCIS*, Montréal, Canada, to be held July, 2004.